

Diffusive sampling for the validation of urban dispersion models

Sotiris VARDOULAKIS^{1,2}, Norbert GONZALEZ-FLESCA¹, Bernard FISHER³,
and Koulis PERICLEOUS²

¹*Institut National de l'Environnement Industriel et des Risques (INERIS)
Parc Technologique ALATA, BP 2, 60550 Verneuil-en-Halatte, France
Tel: +33 3 44 55 64 12, Fax: +33 3 44 55 63 02, sotiris.vardoulakis@ineris.fr*

²*University of Greenwich
School of Computing and Mathematical Science
Maritime Greenwich, University Campus, 30 Park Row, London SE10 9LS, UK*

³*Environment Agency
National Centre for Risk Analysis & Options Appraisal,
Steel House 11 Tothill Street, London SW1H 9NF, UK*

Abstract: Although widely used in workplace, indoor and ambient air quality assessments, diffusive sampling has not yet been established as a common tool for dispersion model validation. In this study, three mathematical models (STREET, OSPM and AEOLIUS) that are likely to be used for regulatory purposes were validated against experimental data obtained in two street canyons in Paris. Diffusive tubes were used to sample a wide range of traffic-related organic compounds at different heights and distances from the kerb. Model input information (site geometry, meteorological and traffic data) was obtained from the competent authorities and compared with on site observations. An algorithm describing vertical pollutant dispersion and an empirical relationship between CO and benzene were used. Diffusive sampling might be seen as a practical and cost-effective method for creating data sets for dispersion model validation.

Keywords: Model validation; Diffusive sampling; Street canyon; Benzene

1. Introduction

Nowadays, several street canyon models of different levels of sophistication are commonly used by local authorities, air quality networks, and research institutions in Europe. Most of these models have been parameterised and validated against real time measurements obtained from roadside monitoring stations.

However, these on-site continuous measurements do not reflect the strong spatial variability of traffic pollution revealed by a number of recent studies [1,2]. This variability, which might have serious implications in terms of population exposure, can be efficiently monitored using diffusive sampling. Furthermore, it may be predicted reliably by adequately validated dispersion models.

Diffusive sampling has become a popular method for assessing air quality due to a number of practical advantages (e.g. no need for power supply, portability of samplers, etc.) Although widely used in workplace, indoor and ambient air quality studies [3,4], it has not yet been established as a common tool for the validation of dispersion models.

The objective of this paper is to present a model validation method involving multisite diffusive sampling. This method was applied to three street canyon models (STREET, OSPM and AEOLIUS) that were validated against experimental data obtained at two different urban sites in Paris, France.

2. Experimental

2.1. Monitoring sites and equipment

Two air quality monitoring campaigns were conducted in street canyons in Paris during winter (Bd. Voltaire, December 1998) and summer (Rue de Rennes, July 1999). The two sites were busy four-lane streets with large pavements and uniform buildings lining up continuously on both sides. The height-to-width (H/W) ratios for Bd. Voltaire and Rue de Rennes were approximately equal to 0.8 and 1.1, and the average traffic volumes during measurements were 30,000 and 23,000 veh/day, respectively.

Active (i.e. pumped) and "passive" (i.e. diffusive) tubes were used in both the canyons to sample benzene, toluene, xylenes (BTX) and other volatile organic compounds (VOC). CO, NO_x and O₃ were continuously monitored using infrared, chemiluminescence and ultra-violet analysers, respectively. Local meteorological parameters were measured at street level and compared with synoptic weather information obtained from a permanent monitoring station located in Montsouris park, within a few km distance of the experimental sites. Hourly traffic volumes and average vehicle speeds were obtained from automatic counters operating in both the streets. Finally, the vehicle fleet composition was estimated from visual observation.

2.2. Diffusive sampling and analysis

Whilst active sampling was conducted only at one kerbside location in each canyon (height of inlet: 3.7 and 2.9 m in Bd. Voltaire and Rue de Rennes respectively), diffusive samplers were placed at several roadside and background locations, at different heights and distances from the kerb.

In Bd. Voltaire, diffusive tubes were located at two different heights (1st and 5th floor) near the walls of the canyon, and at one background site (Fig. 1). The devices remained exposed to ambient concentrations for five days. In Rue de Rennes, two different sets of diffusive tubes were used to examine separately BTX levels during weekend and working weekdays. A more detailed spatial resolution was obtained by increasing the number of sampling locations. In this case, apart from measurements near the walls of the canyon, samples were also taken on the kerbside ($h=1.5$ m), and at two different background sites (Fig. 2).

The diffusive sampling was carried out using combination Radiello/Perkin-Elmer tubes filled with Carbotrap-B and sheltered in aluminium boxes [5]. After recovery from the tubes with thermal desorption, VOCs were analysed in the laboratory using gas chromatography (column type: CP-SIL 5CB, 50 m×0.32 mm, 1.2 μm) and FID. A quality assurance programme, including sampling duplicates and blanks was followed during sampling and analysis.

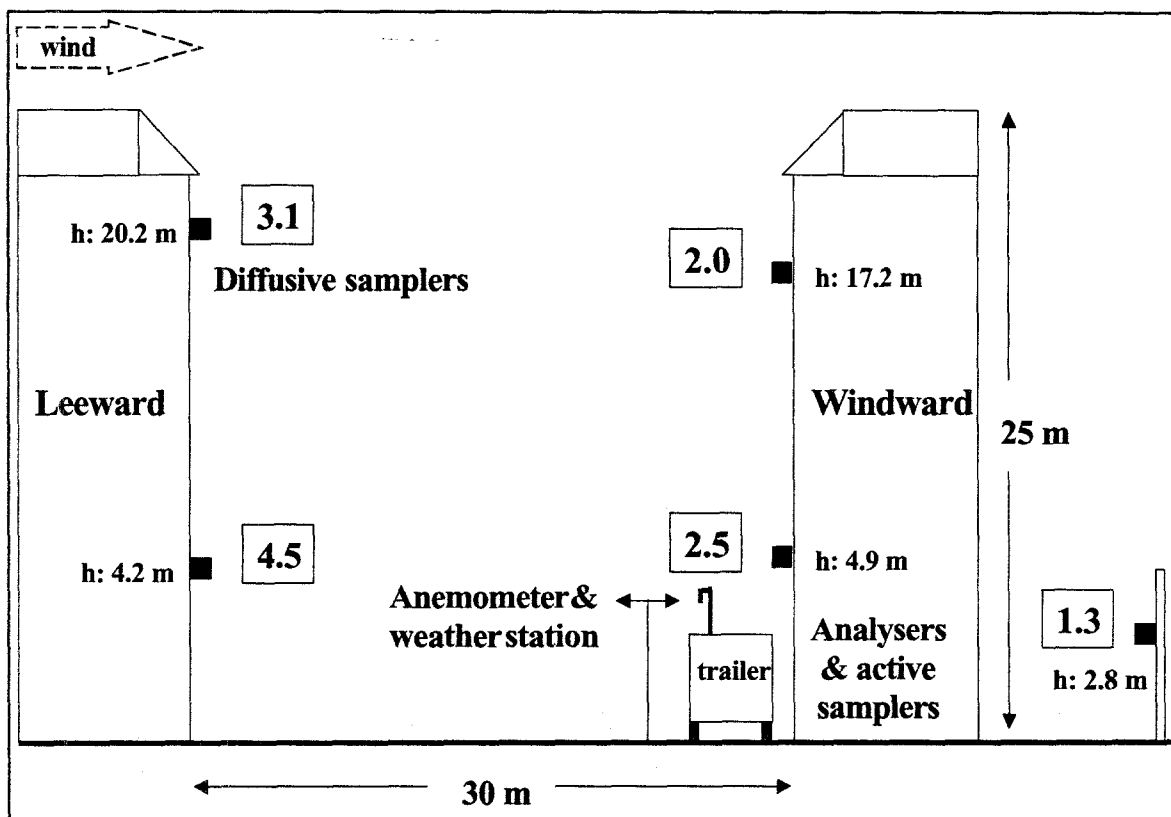


Fig. 1: Diffusive sampling in Bd. Voltaire (14-18 December 1998)

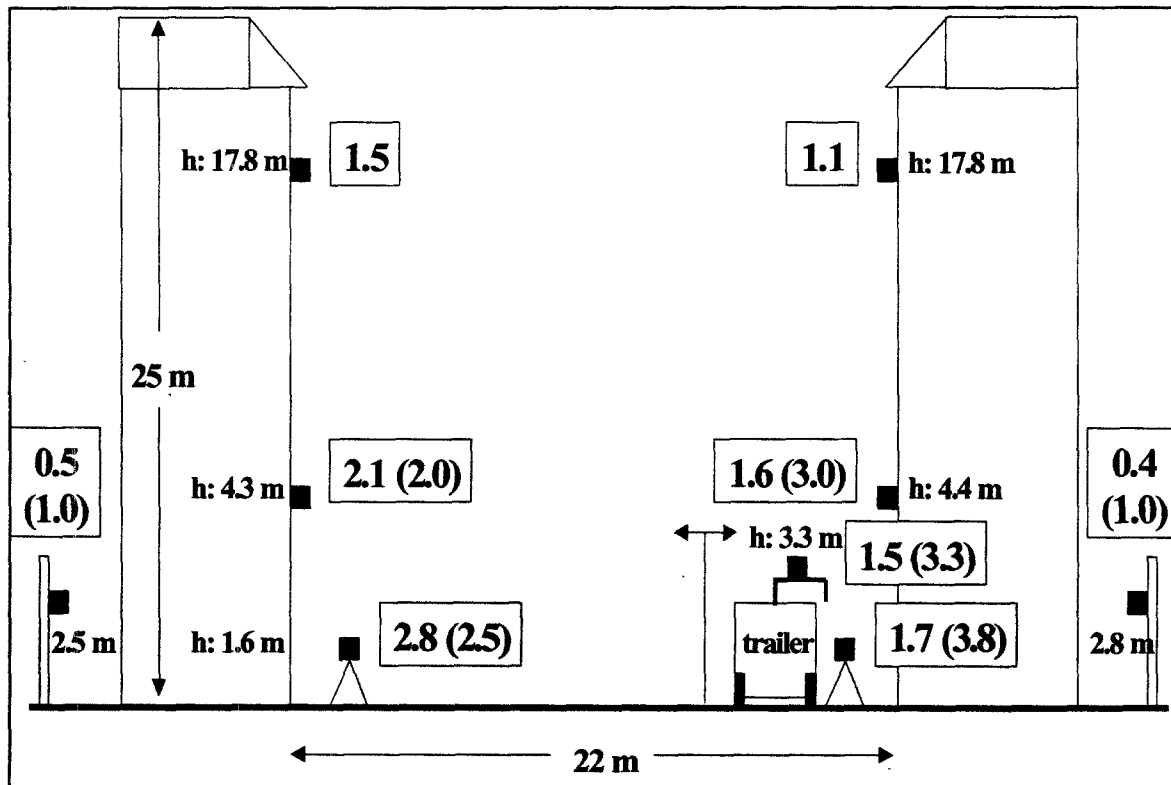


Fig. 2: Diffusive sampling in Rue de Rennes during weekdays (19-23 July) and a weekend (16-18 July 1999, values in parenthesis).

3. Modelling

Three mathematical models, STREET, OSPM, and AEOLIUS, were used for the simulation of pollutant dispersion within the canyons. These relatively simple models (or variations of them) are likely to be involved in a variety of applications including air quality and traffic management, urban planning, population exposure studies, etc.

STREET [6,7] is a box model that uses two different empirical algorithms to reproduce CO concentrations on either side (i.e. leeward and windward) of a street canyon. When the wind direction is parallel or near-parallel to the axis of the canyon, concentrations on the two opposite sides of the street become equal and they are calculated by averaging the results from the two algorithms. The final CO values are obtained by adding the urban background contribution to the kerbside concentrations.

OSPM [8] is a semi-empirical code, which was evolved from the CPBM model [9]. It is designed to produce series of hourly pollutant concentrations at a single receptor location on either side of a street canyon. It assumes three different contributions to the kerbside levels: (a) the contribution from the direct flow of pollutants from the source to the receptor, (b) the recirculation contribution due to the flow of pollutants around an horizontal wind vortex generated within the so called recirculation zone of the canyon, and (c) the urban background contribution. The direct component is calculated applying Gaussian dispersion theory, while a box model algorithm gives the recirculation component. On the leeward side of the street, concentrations are calculated as the sum of the direct and recirculation contributions, while on the windward side, only the direct contribution of emissions generated outside the recirculation zone are taken into account. If the recirculation zone extends throughout the whole canyon, then the windward concentrations are calculated from only the recirculation component. When the wind speed is near zero or parallel to the street axis, the concentrations on both sides of the canyon become equal.

These two models, STREET and OSPM, have been used in many scientific and engineering applications [10,11]. AEOLIUS is a more recent model based on the same formulation as OSPM and mainly used in the U.K. [12].

In STREET, the user externally defines the height (z) of the receptor and its distance from the kerb. By contrast, OSPM and AEOLIUS produce pollutant concentrations only at street level (≈ 2 m), without giving the user the possibility of choosing the height of the receptors. This limitation was overcome by introducing an algorithm that enables the user to establish vertical pollution profiles in the street [13]:

$$C(z) = C_r \exp\left(-\frac{z - z_r}{H}\right) \quad (1)$$

where C_r is the concentration of the pollutant at a reference height z_r on either side of the canyon (H : height of the canyon). Furthermore, an empirical relationship was introduced, so as to allow the calculation of benzene concentrations from CO predictions:

$$\text{Benzene (ppb)} = a \cdot \text{CO (ppm)} \quad (2)$$

The proportionality constant, a , was derived experimentally from simultaneous BTX and CO measurements in both the canyons (3.8 and 3.7 in Bd. Voltaire and Rue de Rennes, respectively).

As inputs, all three models required synoptic wind information, traffic and emission data, as well as the dimensions of the canyons. The rate of release of CO in the street was calculated from hourly traffic volumes and emission factors, which were derived from the site-specific vehicle fleet composition [14]. The relative pollutant contributions from the street and the background were derived from diffusive benzene measurements.

4. Results and discussion

STREET, OSPM and AEOLIUS were initially used to simulate hourly CO averages in Bd. Voltaire and Rue de Rennes. The results showed a good agreement with the continuous CO measurements in both the streets [13,15]. In the present study, the three models were further validated against diffusive benzene measurements.

Applying the empirical relationship (2) to the CO concentrations calculated with STREET, average benzene values were produced for different receptor locations in the street over the diffusive sampling periods (i.e. 2 to 5 day averages) and added to the observed background concentrations. The comparison of the total calculated values with the observations showed a very good general agreement for Rue de Rennes (Fig. 3a), although the model seemed to slightly under-predict the low concentrations observed near the top of the canyon. For Bd. Voltaire, the model under-predicted all measured values (Fig. 3b).

Furthermore, relationship (1) was used to calculate CO concentrations at receptor heights corresponding to the diffusive sampling locations in Bd. Voltaire and Rue de Rennes, using the street level OSPM and AEOLIUS outputs as reference values. Applying relationship (2), average benzene values were obtained and added to the observed background concentrations. Despite some slight under-predictions in the case of Bd. Voltaire, OSPM¹ reproduced successfully the concentration profiles detected in the two canyons (Fig. 3c and 3d). AEOLIUS¹ gave also very good predictions for Rue de Rennes (Fig. 3e), but under-predicted the values observed in Bd. Voltaire (Fig. 3f).

The tendency of all three models¹ to under-predict pollutant concentrations in the case of Bd. Voltaire (i.e. the models under-predicted the CO concentrations from which the benzene averages were calculated) might be attributed to under-estimated CO emissions in this street. More diffusive benzene measurements from other urban canyons are needed for further validating the models as well as the empirical relationship (1). It should be also emphasised that this expression is not applicable to traffic-related pollutants with very short chemical lifetime, like NO₂, which can be also sampled with diffusive tubes. It has been experimentally demonstrated [16] that NO₂ concentrations may even increase along with height within a street canyon, when the weather conditions favour photochemical activity.

The present study showed how diffusive sampling can be used to test the performance of urban dispersion models at different receptor locations within a street. While high spatial resolution might be achieved using diffusive tubes, the temporal resolution obtained from these measurements is relatively low (e.g. weekly averages). Therefore, the "spatial" validation of the models using diffusive sampling results should be coupled with traditional "temporal" validation using continuous monitoring data (e.g. hourly CO averages).

¹ It refers to the model as it was applied in this occasion, i.e. together with expression (1)

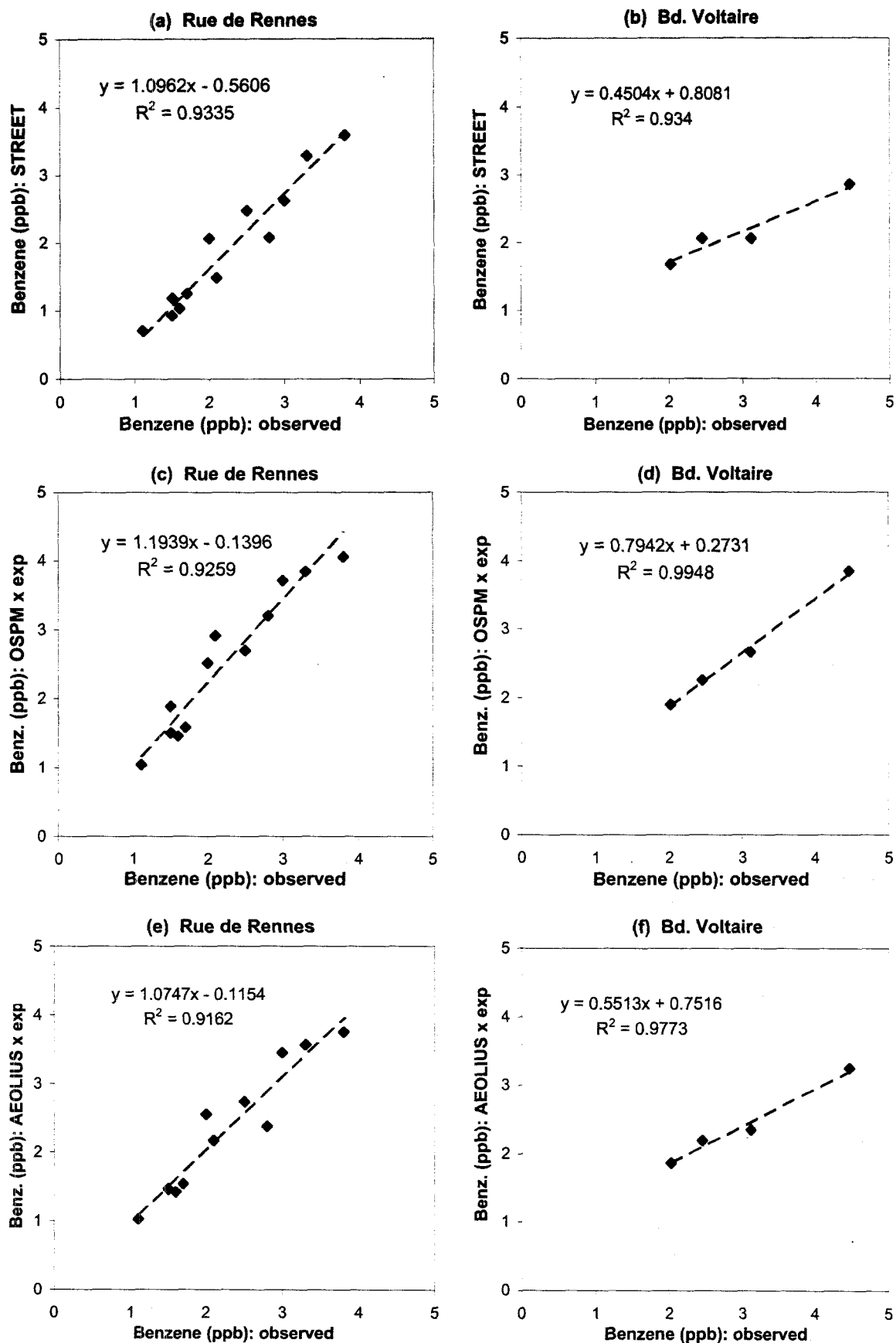


Fig. 3: STREET, OSPM and AEOLIUS predictions vs. observed benzene concentrations obtained with diffusive sampling in Rue de Rennes and Bd. Voltaire.

5. Conclusions

This study demonstrated that diffusive sampling can be a useful tool for validating urban dispersion models. Following a relatively simple methodology, three mathematical models (STREET, OSPM and AEOLIUS) were validated against multisite benzene measurements obtained in two street canyons in Paris. This methodology involved the use of two empirical relationships: the first one for reproducing vertical pollution profiles using street level concentrations, and the second one for calculating benzene values from CO predictions. All three models gave very satisfactory benzene estimates for Rue de Rennes, but under-predicted (especially STREET and AEOLIUS) the concentrations measured in Bd. Voltaire.

The three models, STREET, OSPM and AEOLIUS, had already been validated in the past against continuous measurements from urban air quality monitoring stations. In the present study, the main advantage of using diffusive sampling was that it enabled us to test the models for different receptor locations within the same street. Most importantly, that was achieved without investing a great amount of resources (e.g. sophisticated instrumentation, power supply, etc.) For this reason, it is believed that diffusive sampling will be increasingly used in the future as an alternative technique for creating data sets for model validation.

Acknowledgements

The authors would like to thank Armelle FREZIER (INERIS) for the chemical analysis of the samples, Jean-Claude PINARD (INERIS) for his technical assistance, Mairie de Paris (Direction de la Voirie) for the traffic data furnished, and Dr. R. BERKOWICZ (NERI) for providing and discussing OSPM.

References

- [1] Monn Ch., Carabias V., Junker M., Waeber R., Karrer M., Wanner H.U., 1997. Small-scale spatial variability of particulate matter < 10 μm (PM₁₀) and nitrogen dioxide (NO₂). *Atmospheric Environment* 31 (15), 2243-2247.
- [2] Monn C., 2001. Exposure assessment of air pollutants: a review on spatial heterogeneity and indoor/outdoor/personal exposure to suspended particulate matter, nitrogen dioxide and ozone
- [3] Gonzalez-Flesca N., Bates M., Delmas V., Cocheo V., 2000. Benzene exposure assessment at indoor, outdoor and personal levels. The French contribution to the LIFE MACBETH programme. *Environmental Monitoring and Assessment* 65, 59-67.
- [4] Gonzalez-Flesca N., Vardoulakis S., Cicolella A., 2001. BTX concentrations near a Stage II implemented petrol station. *Environmental Science & Pollution Research*, 8.
- [5] Bates M., Gonzalez-Flesca N., Cocheo V., Sokhi R., 1997. Ambient volatile organic compound monitoring by diffusive sampling. Compatibility of high uptake rate samplers with thermal desorption. *The Analyst* 122, 1481-1484.
- [6] Johnson W.B., Ludwig F.L., Dabberdt, Allen R.J., 1973. An urban diffusion simulation model for carbon monoxide. *Journal of the Air Pollution Control Association* 23, 490-498.
- [7] Dabberdt W.F., Ludwig F.L., Johnson W.B., 1973. Validation and applications of an urban diffusion model for vehicular pollutants. *Atmospheric Environment* 7, 603-618.
- [8] Hertel O., Berkowicz R., 1989. Modelling pollution from traffic in a street canyon. Evaluation of data and model development. NERI, Roskilde, Denmark.
- [9] Yamartino R.J., Wiegand G., 1986. Development and evaluation of simple models for the flow, turbulence and pollutant concentration fields within an urban street canyon. *Atmospheric Environment* 20, 2137-2156.
- [10] Qin Y., Kot S.C., 1993. Dispersion of vehicular emission in street canyons, Guangzhou city, South China (P.R.C.) *Atmospheric Environment* 27B (3), 283-291.
- [11] Kukkonen J., Valkonen E., Walden J., Koskentalo T., Aarnio P., Karppinen A., Berkowicz R., Kartastenpää R., 2001. A measurement campaign in a street canyon in Helsinki and comparison of results with predictions of the OSPM model. *Atmospheric Environment* 35, 231-243.

- [12] Buckland A.T., 1998. Validation of a street canyon model in two cities. *Environmental Monitoring and Assessment* 52, 255-267.
- [13] Vardoulakis S., Gonzalez-Flesca N., Fisher B.E.A., 2001, Assessment of traffic-related air pollution in two street canyons in Paris: implications for exposure studies, *Atmospheric Environment* (in the press).
- [14] Buckland A.T., Middleton D.R., 1999. Nomograms for calculating pollution within street canyons. *Atmospheric Environment* 33, 1017-1036.
- [15] Vardoulakis S., Gonzalez-Flesca N., Fisher B.E.A., 2000. Air quality monitoring and modelling techniques for street canyons: the Paris experience. *Eight International Conference on Air Pollution*, Cambridge, UK, WIT Press, 505-513.
- [16] Väkevä M., Hämeri K., Kulmala M., Lahdes R., Ruuskanen J., Laitinen T., 1999. Street level versus rooftop concentrations of submicron aerosol particles and gaseous pollutants in an urban street canyon. *Atmospheric Environment* 33, 1385-1397.